



Determination of substituting elements environment in LLZO garnet structure by Anomalous X-Ray scattering (AXS).

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キーワード : AXS, Batteries.

1. 背景と研究目的

Materials for solid electrolytes in batteries are an active field of research. Since the first study around 2007, $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) attracted much scientific attention as a solid electrolyte for 'Beyond Li-Ion Battery' concepts such as Li-air and Li-S batteries. The implementation of LLZO as a solid-state electrolyte requires the stabilization of the cubic phase with higher Li-ion conductivity with respect to the tetragonal phase.

The strategy to stabilize the cubic phase is mainly based in cationic substitution. In our case, we introduced Zr, Ce, Hf, Sn, Nb, Sb, and Ta. AXS is a powerful tool to determine the each cation in the lattice.

2. 実験内容

8 samples with composition $\text{Li}_7(\text{La Ce, Hf, Sn, Nb, Sb, Ta})_3\text{Zr}_2\text{O}_{12}$ were measured close to the Hf (9.56 keV) and Ta (9.88 keV) edge in transmission mode using 0.1 mm capillary.

3. 結果および考察

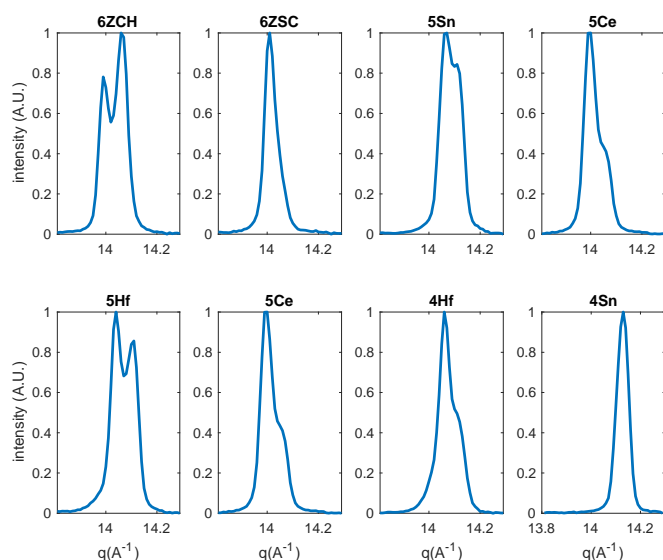


Fig 1 Diffraction patterns of LLZO, with different compositions

All the samples showed the LLZO reported structure as previously confirmed using conventional XRD in the lab.

It is remarkable that almost all samples exhibited a certain type of tetragonal distortion. This result was not observed in the previous measurements at higher energy (17 and 19keV).

The sample 4Sn showed a diffraction pattern in agreement with a cubic structure or at least a tetragonal distortion not possible to distinguish with the present instrumental configuration.

Analysis of the Anomalous Diffraction effect is under analysis.

4. 参考文献

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